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On the connection between transformations in classical mechanics and in quantum mechanics and the phase space representation of quantum mechanics[1]

By U. Uhlhorn

1. Introduction and summary

Classical dynamics may be regarded as a theory of canonical transformations in the phase space (compare the exposition by Tietz [17]), quantum dynamics as a theory of unitary transformations in the state-vector space. The transformation groups of classical and of quantum mechanics are not isomorphic but they contain subgroups which are isomorphic. The classical point transformations can also be represented by unitary transformations in the vector space $\mathcal{A}_1$ (the set of complex-valued phase functions) and the corresponding quantum mechanical transformations can be represented by unitary transformations in the vector space $\mathcal{A}_2$ (the set of linear operators in the state-vector space). According to the quantization prescriptions the vector spaces $\mathcal{A}_1$ and $\mathcal{A}_2$ are isomorphic and can thus be regarded as different representations of the same abstract vector space $\mathcal{A}$. So far the choice of the unitary representations of the dynamical groups is rather ambiguous but if it is required that a certain subgroup should be common to both representations, the transformation connecting the vector spaces $\mathcal{A}_1$ and $\mathcal{A}_2$ is determined nearly completely. This makes it possible to obtain the group of transformations against which the quantization is invariant, and to treat quantum mechanical problems in "phase-space representation".

2. Classical mechanics as a theory of unitary transformations in $\mathcal{A}_1$

In the $2n$-dimensional real space $R_{2n}=\{p_1 \dots p_n, q_1 \dots q_n \mid -\infty < p_\nu, q_\nu < \infty\}$[2] (the phase space) consider the continuous group $\mathfrak{c}$ of canonical transformations which map R_{2n} on itself. This means that the introduction of periodic coordinates (e.g. polar coordinates in configuration space) is excluded. Thus $\mathfrak{c}$ is a subgroup of the complete group of canonical transformations. According to

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[1] Presented, in shortened form, at the Conference of Physicists, Stockholm, September 1955.

[2] The following notations will be used frequently:

$$p=(p_1 \dots p_n),\ q=(q_1 \dots q_n);\ p\cdot q=\sum_1^n p_\nu q_\nu$$

$$d(p,q)=d p_1 \dots d p_n\, d q_1 \dots d q_n.$$

Sophus Lie [9] it is possible to find, corresponding to any element α of $\mathfrak{c}$, a generating real function $a(p, q)$ so that

$$\left.\begin{aligned} \alpha^{-1} p_\nu &= p_\nu + \lambda (a, p_\nu) + \frac{\lambda^2}{2!} (a, (a, p_\nu)) + \cdots{}^1 \\ \alpha^{-1} q_\nu &= q_\nu + \lambda (a, q_\nu) + \frac{\lambda^2}{2!} (a, (a, q_\nu)) + \cdots . \end{aligned}\right\} \quad (1)$$

Here

$$(X, Y) = \sum_1^n \left(\frac{\partial X}{\partial q_\nu} \frac{\partial Y}{\partial p_\nu} - \frac{\partial X}{\partial p_\nu} \frac{\partial Y}{\partial q_\nu} \right)$$

is the Poisson bracket and λ is a real number. If the operator

$$\mathcal{D}[a] = i \sum_1^n \left(\frac{\partial a}{\partial q_\nu} \frac{\partial}{\partial p_\nu} - \frac{\partial a}{\partial p_\nu} \frac{\partial}{\partial q_\nu} \right)$$

is introduced the equations (1) can be summed up in the operator relation

$$\alpha^{-1} = e^{\lambda \frac{1}{i} \mathcal{D}[a]}. \quad (2)$$

In the vector space $\mathcal{A}_1$ consisting of all complex-valued functions which are infinitely many times differentiable in R_{2n}, the inner product of any two elements $f(p, q)$ and $g(p, q)$ may be defined as

$$(f|g) = \int\int f(p, q)^* g(p, q) \frac{1}{h^n} d(p, q). \quad (3)$$

Planck's constant h is introduced only to get agreement with the corresponding expression in quantum mechanics (compare Section 3). The integral (3) is not convergent for every choice of elements from $\mathcal{A}_1$ but it is certainly convergent if the two vectors belong to the Hilbert subspace $\mathcal{A}_{1H}$ which is defined as the subspace of $\mathcal{A}_1$ which contains all elements with finite norm: $(f|f) < \infty$. $\mathcal{A}_{1H}$ is dense in $\mathcal{A}_1$ and hence any element of $\mathcal{A}_1$ may be approximated by an element of $\mathcal{A}_{1H}$.

The group $\mathfrak{c}$ of point transformations induces in $\mathcal{A}_1$ a group $\mathfrak{C}$, isomorphic to $\mathfrak{c}$, of linear transformations defined by

$$\Gamma_\alpha f(p, q) = f(\alpha^{-1} p, \alpha^{-1} q), \quad (4)$$

where α is any element of $\mathfrak{c}$ and Γ_α the corresponding element of $\mathfrak{C}$. The inner product (3) is invariant against $\mathfrak{C}$ owing to the well-known fact that the Jacobian of a canonical point transformation is equal to one. Thus $\mathfrak{C}$ is a unitary group in $\mathcal{A}_1$. From (4) it follows immediately that algebraic relations and reality properties are invariant against $\mathfrak{C}$. If α^{-1} is the point transformation in

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[1] α^{-1} denotes the inverse transformation of α. The definition in terms of α^{-1} is chosen for convenience only.

(2) the unitary transformation in $\mathcal{A}_1$ corresponding to α can be written $\Gamma_\alpha = \exp(\lambda [1/i] \mathcal{D}[a])$ which means that for any element f of $\mathcal{A}_1$

$$\Gamma_\alpha f(p, q) = e^{\lambda \frac{1}{i} \mathcal{D}[a]} f(p, q) = f(\Gamma_\alpha p, \Gamma_\alpha q),$$
$$(\Gamma_\alpha p_\nu = \alpha^{-1} p_\nu, \ \Gamma_\alpha q_\nu = \alpha^{-1} q_\nu).$$

This can be proved by induction when use is made of the "distributive" property of the operator $\mathcal{D}[a]$

$$\mathcal{D}[a](f g) = (\mathcal{D}[a] f) g + f \mathcal{D}[a] g.$$

As the transformation $\exp(\lambda [1/i] \mathcal{D}[a])$ is unitary the operator $\mathcal{D}[a]$ must be hermitean, i.e. $(f | \mathcal{D}[a] g)^* = (g | \mathcal{D}[a] f)$, which can also be shown by partial integration. To any real element $a(p, q)$ of $\mathcal{A}_1$ there corresponds a hermitean operator $\mathcal{D}[a]$. These operators form an infinite, infinitesimal group and the commutator of any two, $\mathcal{D}[a]$ and $\mathcal{D}[b]$, of them is

$$\frac{1}{i} (\mathcal{D}[a] \mathcal{D}[b] - \mathcal{D}[b] \mathcal{D}[a]) = \mathcal{D}[(a, b)],$$

where (a, b) is again the Poisson bracket of $a(pq)$ and $b(p, q)$, as may easily be shown by direct calculation. The necessary and sufficient condition for $\mathcal{D}[a]$ and $\mathcal{D}[b]$ to commute is thus $(a, b) = \text{constant}$.

As a consequence of this the $2n$ hermitean operators $(\mathcal{D}[p_\nu], \mathcal{D}[q_\nu])$, which correspond to the infinitesimal group of translations in the phase space, form a commuting set. The set is also complete in $\mathcal{A}_{1H}$. The eigenfunctions are determined from the equations

$$\mathcal{D}[p_\nu] \psi(p, q) = -i \frac{\partial}{\partial q_\nu} \psi(p, q) = x_\nu \psi(p, q)$$

$$\mathcal{D}[q_\nu] \psi(p, q) = \quad i \frac{\partial}{\partial p_\nu} \psi(p, q) = y_\nu \psi(p, q).$$

A normalized solution is

$$(p, q | x, y) = \hbar^{n/2} e^{i(x \cdot q - y \cdot p)}. \tag{5}$$

The solution is unique as to an arbitrary phase factor. With the notation $(p, q | x, y)^* = (x, y | p, q)$ the ortho-normality and completeness relations read

$$\iint (x, y | p, q) \frac{d(p, q)}{h^n} (p, q | x', y') = \delta(x - x') \delta(y - y'),$$

$$\iint (p, q | x, y) \, d(x, y) \, (x, y | p', q') = h^n \delta(p - p') \delta(q - q').$$

Any element f of $\mathcal{A}_{1H}$ may be expanded in terms of the eigenfunctions (5):

$$f(p, q) = \iint (p, q | x, y) \, d(x, y) \, (x, y | f)$$

where

$$(x, y \mid f) = \iint (x, y \mid p, q)\, f(p, q)\, \frac{d(p, q)}{h^n}.$$

The transformation $T f(p, q) = (x, y \mid f)$ is obviously unitary.

Consider now a mechanical system of n degrees of freedom. In classical mechanics physical observables are represented by real phase functions and states (pure cases) of the system are represented by points in the phase space. For our purpose it is, however, more convenient to adopt the general formalism of statistical mechanics (Gibbs [5]). The state, which may then be either a pure case or a mixture, is represented by a distribution ϱ, i.e. a completely additive, non-negative set-function, in the phase space. This means that to every subspace of R_{2n} there corresponds a real number which is the measure of probability for the given subspace. The distribution need not have a density-in-phase $\varrho(p, q)$, but if the formalism of L. Schwarz [13] is applied it is possible to treat, in a consistent way, the distribution ϱ itself as if it were the density. This formalism then also includes the pure case. A state represented by ϱ is pure with respect to an observable $a(p, q)$ if $a(p, q)\, \varrho = a'\, \varrho$ (a' = real number). E.g. the microcanonical distribution of Gibbs is pure with respect to the total energy. If the distribution is normalized to unity the expected value of an observable $a(p, q)$ in the state represented by ϱ is the Stieltjes integral $(\varrho \mid a) = \iint d\varrho\, a(p, q)\, (1/h^n)$.

The equation of motion may be written as a differential equation for a unitary operator $\Gamma(t)$ belonging to the group $\mathbb{C}$

$$\frac{1}{i} \mathcal{D}[H]\, \Gamma(t) = \frac{d}{dt} \Gamma(t), \quad \Gamma(0) = 1$$

where $H = H(p, q, t)$ is the Hamiltonian of the system. Alternatively the time dependence may be attributed to the state of the system (Schrödinger picture of classical mechanics)

$$\varrho_t = \Gamma(t)\, \varrho \text{ corresponding to } \frac{\partial \varrho_t}{\partial t} = (H, \varrho_t)$$

or to the observables (Heisenberg picture of classical mechanics)

$$a_t(p, q) = \Gamma(t)^{-1} a(p, q) = a(\Gamma(t)^{-1} p, \Gamma(t)^{-1} q) = a(p_t, q_t)$$

corresponding to

$$\frac{\partial}{\partial t} a_t(p, q) = \frac{d}{dt} a(p_t, q_t) = \sum_{=1}^{n} \left(\frac{\partial a}{\partial q_{t\nu}} \frac{\partial H}{\partial p_{t\nu}} - \frac{\partial a}{\partial p_{t\nu}} \frac{\partial H}{\partial q_{t\nu}} \right)$$

in complete analogy to the case in quantum mechanics. For the proof of the last relation it is essential that the Poisson brackets are invariant against the transformation group $\mathbb{C}$.

3. Quantum mechanics as a theory of unitary transformations in $\mathcal{A}_2$. The correspondence between $\mathcal{A}_1$ and $\mathcal{A}_2$

In quantum mechanics observables are represented by linear hermitean operators in an extended (in accordance with the definition of Dirac [2]) Hilbert space Hi (the state-vector space). The extension means that Hi contains also vectors which are not normalizable. The state of a physical system (which may be a pure case or a mixture) is represented by a hermitean non-negative operator ϱ, the statistical operator of J. v. Neumann [10, 11] (see also Dirac [2]). If ϱ is normalized (i.e. $Sp\,\varrho = \int \langle m|\varrho|m\rangle\, d(m) = 1$, where $\{|m\rangle\}$ is some complete orthonormalized set in Hi) the expected value of an observable A is $Sp\,\varrho A = \iint \langle n|\varrho|m\rangle^* \langle n|A|m\rangle\, d(n,m)$. The state represented by ϱ is pure if the normalized ϱ is a projection operator: $\varrho^2 = \varrho$. In general $\varrho - \varrho^2 \geq 0$, i.e. $\varrho - \varrho^2$ is a non-negative operator.

Instead of regarding the space Hi formed by the state vectors we now consider the vector space $\mathcal{A}_2$ formed by all linear operators in Hi. The inner product of two elements A and B of $\mathcal{A}_2$ may be defined as

$$(A|B) = Sp\,A^* B = \iint \langle m|A|n\rangle^* \langle m|B|n\rangle\, d(m,n)^1. \tag{6}$$

The dynamical group of transformations $\mathbf{u}$ of quantum mechanics is the group of unitary transformations in Hi. To any element U of $\mathbf{u}$ (which is contained in $\mathcal{A}_2$) it is possible to find a generating hermitean operator S so that $U = \exp\,([\lambda/i\hbar]\,S)$ where λ is a real number (Stone [15]). The group $\mathbf{u}$ induces in $\mathcal{A}_2$ a group of transformations $\mathbf{U}$ (unitary similarity transformations) defined by

$$\Lambda_u A = U A U^{-1}$$

for any $A \in \mathcal{A}_2$ where $U \in \mathbf{c}$ and Λ_u is the corresponding element of $\mathbf{U}$. Obviously the inner product (6) is invariant against $\mathbf{U}$ which is thus a unitary group. Algebraic relations and reality properties are also invariant against $\mathbf{U}$.

If S is any hermitean operator in Hi and A any element of $\mathcal{A}_2$

$$\mathcal{H}[S]\,A = \frac{1}{\hbar}(SA - AS) \tag{7}$$

defines a hermitean operator $\mathcal{H}[S]$ in $\mathcal{A}_2$ for

$$(A|\mathcal{H}[S]\,B)^* = Sp\left\{A^* \frac{1}{\hbar}(SB - BS)\right\} = (B|\mathcal{H}[S]\,A).$$

All the operators of the type (7) form an infinitesimal group. The commutator of two operators $\mathcal{H}[S]$ and $\mathcal{H}[T]$ is

$$\frac{1}{i}(\mathcal{H}[S]\,\mathcal{H}[T] - \mathcal{H}[T]\,\mathcal{H}[S]) = \mathcal{H}\left[\frac{1}{i\hbar}(ST - TS)\right]\cdot$$

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[1] A^* denotes the hermitean conjugate of A.

Thus $\mathcal{H}[S]$ and $\mathcal{H}[T]$ commute if and only if $(1/i\hbar)(ST-TS)=\text{constant } 1$. The transformation Λ_u of **U** corresponding to $U=\exp(\lambda[1/i\hbar]S)$ may now be written

$$\Lambda_u = e^{\lambda \frac{1}{i} \mathcal{H}[S]}.$$

In order to obtain a correspondence between the vector spaces $\mathcal{A}_1$ and $\mathcal{A}_2$ we make use of the following quantization prescriptions:

a) $\mathcal{A}_1$ and $\mathcal{A}_2$ are isomorphic vector spaces, i.e. if $f(pq) \leftrightarrow f_{\text{op}}$ and $g(p,q) \leftrightarrow g_{\text{op}}$ then:

$$\alpha f(p,q) + \beta g(p,q) \leftrightarrow \alpha f_{\text{op}} + \beta g_{\text{op}} \quad (\alpha \text{ and } \beta, \text{ complex numbers}).$$

b) Real functions correspond to hermitean operators, i.e. if $f(p,q) \leftrightarrow f_{\text{op}}$ then $f^*(p,q) \leftrightarrow f^*_{\text{op}}$.

c) If $p_\mu \leftrightarrow P_\mu$ and $q_\mu \leftrightarrow Q_\mu$ then

$$\frac{1}{i\hbar}(P_\mu P_\nu - P_\nu P_\mu) = \frac{1}{i\hbar}(Q_\mu Q_\nu - Q_\mu Q_\nu) = 0$$

$$\frac{1}{i\hbar}(Q_\mu P_\nu - P_\nu Q_\mu) = \delta_{\mu\nu} 1.$$

As is well known it follows from the quantization prescriptions (c) that if $F(P,Q)$ is any analytic function of the operators (P,Q) then

$$\mathcal{H}[P_\mu] F(P,Q) = -i \frac{\partial F}{\partial Q_\mu}(P,Q)$$

$$\mathcal{H}[Q_\mu] F(P,Q) = \quad i \frac{\partial F}{\partial P_\mu}(P,Q)$$

and as a direct consequence

$$e^{\frac{\lambda}{i} \mathcal{H}[P_\mu]} F(P,Q) = F(P, Q_\mu - \lambda)$$

$$e^{\frac{\mu}{i} \mathcal{H}[Q_\nu]} F(P,Q) = F(P_\nu + \mu, Q).$$

As a special consequence of this

$$e^{\frac{1}{i\hbar}\lambda\cdot Q} \, e^{\frac{1}{i\hbar}\mu\cdot P} = e^{\frac{1}{i\hbar}\mu\cdot\lambda} \, e^{\frac{1}{i\hbar}\mu\cdot P} \, e^{\frac{1}{i\hbar}\lambda\cdot Q}. \tag{8}$$

It can also be shown (Weyl [18], Groenewold [6]) that

$$e^{\frac{1}{i\hbar}(\mu\cdot P+\lambda\cdot Q)} = e^{\frac{1}{i\hbar}\frac{\mu\cdot\lambda}{2}} \, e^{\frac{1}{i\hbar}\mu\cdot P} \, e^{\frac{1}{i\hbar}\lambda\cdot Q}.$$

The $2n$ hermitean operators $\mathcal{H}[P_\mu]$, $\mathcal{H}[Q_\mu]$ form a complete commuting set in $\mathcal{A}_{2H}$ (the Hilbert subspace of $\mathcal{A}_2$). A normalized solution of the corresponding eigenvalue equations

$$\mathcal{H}[P_\mu]\,\phi = x_\mu\,\phi$$

$$\mathcal{H}[Q_\mu]\,\phi = y_\mu\,\phi$$

is obviously given by

$$\hbar^{n/2}\,e^{-i\,y\cdot P}\,e^{i\,x\cdot Q}. \tag{9}$$

The solution is unique as to an arbitrary phase factor. Any element A of the Hilbert subspace $\mathcal{A}_{2H}$ of $\mathcal{A}_2$ can be expanded in terms of the eigenvectors $\phi(x, y)$ of $\mathcal{H}[P_1] \dots \mathcal{H}[Q_n]$:

$$A = \iint \phi(x, y)\, d(x, y)\,(x, y \mid A) \tag{10}$$

where

$$(x, y \mid A) = Sp\,\phi(x, y)^*\,A = (\phi(x, y) \mid A).$$

If the phase factor of $\phi(x, y)$ is chosen as in (9) the expansion (10) is well ordered in the sense of Dirac [4] and Jordan [8], i.e.

$$\langle P' \mid A \mid Q' \rangle = \iint \hbar^{n/2}\,e^{-i\,y\cdot P' + i\,x\cdot Q'}\,d(x, y)\,(x, y \mid A)$$

P', Q' being eigenvalues of P and Q.

From the quantization prescriptions (c) it follows that the infinitesimal groups generated by $\mathcal{D}[p_1], \dots \mathcal{D}[q_n]$ in $\mathcal{A}_1$ and by $\mathcal{H}[P_1], \dots \mathcal{H}[Q_n]$ in $\mathcal{A}_2$ are isomorphic[1] (compare v. Hove [7]) and according to the prescriptions (a) $\mathcal{A}_1$ and $\mathcal{A}_2$ can be regarded as different representations of the same abstract vector space $\mathcal{A}$. Thus it must be possible to represent the two infinitesimal groups by the same transformation group in $\mathcal{A}$. When this is done the transformation connecting the representations $\mathcal{A}_1$ and $\mathcal{A}_2$ is determined, for as

$$\mathcal{D}[p_1] \leftrightarrow \mathcal{H}[P_1], \dots, \mathcal{D}[q_n] \leftrightarrow \mathcal{H}[Q_n],$$

we must have a correspondence between the eigenvectors of the operators and each set of eigenvectors is complete in its vector space. This means that

$$\hbar^{n/2}\,e^{-i\,y\cdot p + i\,x\cdot q} \leftrightarrow \hbar^{n/2}\,R\,e^{i\,\alpha}\,e^{-i\,y\cdot P}\,e^{i\,x\cdot Q}$$

(for all x, y; $R > 0$ constant, α real function of (x, y)). As this shall be true for all (x, y) we get for small (x, y)

$$-iy\cdot p + ix\cdot q \leftrightarrow R\,e^{i\alpha}\{-iy\cdot P + ix\cdot Q\}$$

and according to the quantization prescriptions (a) it follows that $R = 1$ (this is the justification for the appearance of $\hbar$ in the definition (3)). From the prescription (b) we get

$$\alpha(-x, -y) + \alpha(x, y) = x\cdot y\,\hbar.$$

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[1] The isomorphism is due to the one-one correspondence of the commutators (Lie's condition).

With the simplest possible choice: $\alpha(x, y) = (\hbar/2)\, x \cdot y$, we put

$$\phi(x, y) = \hbar^{n/2} e^{i \frac{\hbar}{2} x \cdot y} e^{-iy \cdot P} e^{ix \cdot Q} = \hbar^{n/2} e^{i(-y \cdot P + x \cdot Q)}.$$

With the notations

$$(x, y \,|\, A) = Sp\, \phi(x, y)^* A \quad (A \,|\, x, y)^* = (x, y \,|\, A)$$

we obtain

$$A(p, q) = (p, q \,|\, A) = \iint (p, q \,|\, x, y)\, d(x, y)\, (x, y \,|\, A).$$

Hence the unitary transformation connecting $\mathcal{A}_1$ and $\mathcal{A}_2$ is obtained and the inner products (3) and (6) are really identical. This connection between phase functions and operators was proposed by Weyl from group-theoretical considerations.[1]

As quantum mechanics is usually formulated in configuration-space representation it is of interest to find out the transformation from this representation to the phase-space representation $\mathcal{A}_1$. From the representative

$$\langle Q' \,|\, \phi(x, y) \,|\, Q'' \rangle = \hbar^{n/2} \delta(Q' - Q'' - \hbar y)\, e^{i \frac{\hbar}{2} x \cdot y} e^{ix \cdot Q''}$$

we obtain

$$(p, q \,|\, A) = \left(\frac{2}{\hbar}\right)^n \int\!\!\int \langle q - x \,|\, A \,|\, q + x \rangle\, e^{\frac{2i}{\hbar} p \cdot x}\, d(x)$$

which is identical with a transformation proposed by Dirac in connection with the Thomas Fermi approximation [3] and used by Wigner [20] to obtain the quantum correction for thermodynamic equilibrium.

4. The phase-space representation. Connection between the groups of classical and of quantum mechanics

If A and B are two operators in the state-vector space Hi, the phase-space representative of their product AB may be obtained with the use of (8)

$$\begin{aligned}(p, q \,|\, AB) &= \iiiint e^{\frac{i\hbar}{2}(x \cdot v - y \cdot u)}\, e^{\frac{i\hbar}{2}(x + u) \cdot (y \cdot v)}\, e^{-i(y + v) \cdot P}\, e^{i(x + u) \cdot Q}\, d(x, y, u, v) \\ &= e^{\frac{i\hbar}{2} \sum_{\mu=1}^{n} \left(\frac{\partial}{\partial q'_\mu} \frac{\partial}{\partial p_\mu} - \frac{\partial}{\partial p'_\mu} \frac{\partial}{\partial q_\mu}\right)} (p', q' \,|\, A)\, (p, q \,|\, B) \big|_{p = p' \quad q = q'} \qquad (11) \\ &= (p, q \,|\, A)\, (p, q \,|\, B) + 0(\hbar).\end{aligned}$$

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[1] In this connection it should be remarked that the frequently used prescription for obtaining the operator f_{op} corresponding to a phase function $f(p, q) = \sum_\mu \varphi_\mu(p)\, \psi_\mu(q)$:

$$f_{\mathrm{op}} = \tfrac{1}{2} \sum_\mu (\varphi_\mu(P)\, \psi_\mu(Q) + \psi_\mu(Q)\, \varphi_\mu(P))$$

(Sommerfeld [14], Bopp [1]) is not correct from our standpoint as it corresponds to an expansion in terms of non-normalized eigenvectors $\frac{1}{2}(1 + e^{i\hbar x \cdot y})\, e^{-iy \cdot P} e^{ix \cdot Q}$ which destroys the one-one correspondence between $\mathcal{A}_1$ and $\mathcal{A}_2$.

From (11) one obtains the representatives of the commutator $(1/i\hbar)(AB-BA)$

$$(p,q\,|\,\frac{1}{i\hbar}(AB-BA)) = \frac{2}{\hbar}\sin\left\{\frac{\hbar}{2}\sum_{\mu=1}^{n}\left(\frac{\partial}{\partial q'_\mu}\frac{\partial}{\partial p_\mu}-\frac{\partial}{\partial p'_\mu}\frac{\partial}{\partial q_\mu}\right)\right\}(p',q'\,|\,A)\,(p,q\,|\,B) \qquad (12)$$
$$= ((p,q\,|\,A),\,(p,q\,|\,B)) + 0\,(\hbar^2)$$

and of the anticommutator $\frac{1}{2}(AB+BA)$

$$(p,q\,|\,\tfrac{1}{2}(AB+BA)) = \frac{1}{\hbar}\cos\left\{\frac{\hbar}{2}\sum_{\mu=1}^{n}\left(\frac{\partial}{\partial q'_\mu}\frac{\partial}{\partial p_\mu}-\frac{\partial}{\partial p'_\mu}\frac{\partial}{\partial q_\mu}\right)\right\}(p',q'\,|\,A)\,(p,q\,|\,B)$$
$$= (p,q\,|\,A)\,(p,q\,|\,B) + 0\,(\hbar^2).$$

These expressions can be used for a comparison of the groups **C** and **U**.

Any element of **C** may be written in the form $\exp([\lambda/i]\,\mathcal{D}[a])$, i.e. as a finite or infinite sum of classical Poisson bracket relations

$$e^{\frac{\lambda}{i}\mathcal{D}[a]}\,f = f + \lambda\,(a,f) + \frac{\lambda^2}{2!}\,(a,(a,f)) + \cdots$$

and any element of **U** may be written in the form $\exp([\lambda/i]\,\mathcal{H}[S]$, i.e. as a sum of commutation relations

$$e^{\frac{\lambda}{i}\mathcal{H}[S]}\,A = A + \lambda\,[S,A] + \frac{\lambda^2}{2!}\,[S,[S,A]] + \cdots$$

where $[A,F] = (1/i\hbar)(AF-FA)$. Hence a transformation $\exp([\lambda/i]\,\mathcal{H}[S])$ belonging to **U** also belongs to **C** if and only if the representative of the commutator of S with any element of $\mathcal{A}_2$ is equal to the Poisson bracket of the corresponding representatives:

$$(p,q\,|\,\frac{1}{i\hbar}(SA-AS)) = ((p,q\,|\,S),\,(p,q\,|\,A))$$

and this is true when and only when the expansion of the operator (12) contains only one term. Hence S must be a polynomial in the P and Q of not higher than the second degree

$$S = \sum a_{\varkappa\lambda}P_\varkappa P_\lambda + \tfrac{1}{2}\sum b_{\varkappa\lambda}(P_\varkappa Q_\lambda + Q_\varkappa P_\lambda) + \sum c_{\varkappa\lambda}Q_\varkappa Q_\lambda + \sum d_\varkappa P_\varkappa + \sum e_\varkappa Q_\varkappa + f.$$

The corresponding transformations of $\mathfrak{c}$ are of the form

$$\gamma\,p_\mu = \sum_\nu \alpha_{\mu\nu}\,p_\nu + \sum_\nu \beta_{\mu\nu}\,q_\nu + \sigma_\mu$$
$$\gamma\,q_\mu = \sum_\nu \alpha'_{\mu\nu}\,p_\nu + \sum_\nu \beta'_{\mu\nu}\,q_\nu + \tau_\mu$$

with the real coefficients satisfying

$$\sum_{\varkappa} (\alpha_{\mu\varkappa}\beta_{\lambda\varkappa} - \beta_{\mu\varkappa}\alpha_{\lambda\varkappa}) = 0,$$

$$\sum_{\varkappa} (\alpha'_{\mu\varkappa}\beta'_{\lambda\varkappa} - \beta'_{\mu\varkappa}\alpha'_{\lambda\varkappa}) = 0,$$

$$\sum (\alpha_{\mu\varkappa}\beta'_{\nu\varkappa} - \beta_{\mu\varkappa}\alpha'_{\nu\varkappa}) = \delta_{\mu\nu}.$$

This is the so-called symplectic group, see e.g. Weyl [19]. As a consequence of this the dynamical problem corresponding to a Hamiltonian of oscillator type has the same solution in classical and in quantum mechanics.

The transformations of the symplectic type constitute the group of invariance of the quantization (which is hence a rather restricted one).

However, every transformation of the group **U** induces a point transformation in R_{2n}:

$$\begin{aligned} \gamma_s p_\mu &= (p, q \,|\, e^{\frac{\lambda}{i}\varkappa[S]} P_\mu e^{-\frac{\lambda}{i}\varkappa[S]}), \\ \gamma_s q_\mu &= (p, q \,|\, e^{\frac{\lambda}{i}\varkappa[S]} Q_\mu e^{-\frac{\lambda}{i}\varkappa[S]}). \end{aligned} \tag{13}$$

Evidently any infinitesimal transformation of this type is an infinitesimal canonical point transformation whose generating function is the representative of S. There are, however, some transformations belonging to **U** though not belonging to **C** which induce finite point transformations of type (13) which belong to **c**. The most important transformations of this type are the so-called extended point transformations:

$$\begin{aligned} &Q_\mu \to F_\mu(Q) \\ &P_\mu \to \tfrac{1}{2} \sum_\nu (\varphi_{\mu\nu}(Q) P_\nu + P_\nu \varphi_{\mu\nu}(Q)) \end{aligned}$$

which are generated by hermitean operators of the form

$$\tfrac{1}{2} \sum_1^n (P_\mu f_\mu(Q) + f_\mu(Q) P_\mu).$$

The corresponding transformation in R_{2n} may be written

$$\begin{aligned} &\gamma q_\mu = F_\mu(q) \\ &\gamma p_\mu = \sum_\nu \left(\frac{\partial \psi_\nu}{\partial q_\mu}(\gamma q)\, p_\nu\right) \qquad (\gamma^{-1} q_\mu = \psi_\mu(q)). \end{aligned}$$

Hence there is one subgroup isomorphic to the group of extended point transformations in **C** and one in **U**, but these two subgroups are not identical and the quantization is not invariant against an arbitrary extended point transformation. However, as long as only operators are considered, which are polynomials of second degree in the P and Q, or are of the type

$$\tfrac{1}{2} \sum_{\mu=1}^n p_\mu A_\mu(Q) + A_\mu(Q)\, p_\mu,$$

the quantization is invariant.

5. Phase-space representation of the statistical operator. Determination of stationary states

The expected value of an observable, represented by a phase function $A(p, q)$ or by an operator A in Hi, in a state represented by ϱ may be written

$$(\varrho \,|\, A) = Sp\, \varrho A = \iint \varrho(p, q) \frac{d(p, q)}{h^n} A(p, q)$$

where $\varrho(p, q)$ is the representative of the statistical operator ϱ. This is thus completely the same relation as in the classical case. However, the quantum mechanical distribution in R_{2n}, defined by its density $\varrho(p, q)$, has several properties which distinguish it from the classical distribution. It was mentioned in Section 3 that the operator ϱ satisfies the inequality $\varrho \geq \varrho^2$. Taking the trace we get the equivalent relation

$$1 \geq (\varrho \,|\, \varrho) = \iint \varrho^2(p, q)\, d(p, q) \frac{1}{h^n} \tag{14}$$

and $(\varrho \,|\, \varrho) = 1$ if and only if the state is pure. (Compare Takabayashi [16].) If we assume a distribution, $\varrho(p, q) = k$ when (p, q) is in a set of measure $1/k$ and otherwise $\varrho(p, q) = 0$ we find that $k \leq 1$. Especially $k = 1$ corresponds to a pure state and to the introduction of cells in the phase space in the old quantum theory (e.g. Planck [12]). Hence pure states in the classical sense (Sec. 2) cannot occur at all in quantum mechanics. Evidently this restriction must be related to the Heisenberg inequality and it may in this connection be interesting to make a direct derivation of the distribution of minimum despersion in phase space.

The statistical momenta corresponding to the observables P and Q in the state ϱ may be defined in analogy to ordinary statistics as

$$\alpha_{st} = Sp\,(\varrho P^s Q^t).$$

The central momenta are then given as

$$\mu_{st} = Sp\,(\varrho (P - \alpha_{10})^s (Q - \alpha_{01})^t).$$

The modulus $|r|$ of the coefficient of correlation

$$r = \frac{\mu_{11}}{\sqrt{\mu_{20}\, \mu_{02}}}$$

is never greater than 1. Hence

$$\mu_{20}\, \mu_{02} \geq |\mu_{11}|^2 = \left| Sp\,(\varrho\, \tfrac{1}{2}\, [P, Q]_+) - \frac{i\hbar}{2} \right|^2 \geq \left(\frac{\hbar}{2}\right)^2$$

which contains the Heisenberg inequality. The equality $\mu_{20}\, \mu_{02} = (\hbar/2)^2$ obviously occurs if and only if

$$\eta(P,Q)\,\varrho=0 \quad \text{where} \quad \eta(P,Q)=\frac{P-\alpha_{10}}{\sqrt{\mu_{20}}}-i\,\frac{Q-\alpha_{01}}{\sqrt{\mu_{02}}}. \tag{15}$$

As an immediate consequence of (15) ϱ commutes with the operator

$$A(P,Q)=\left(\frac{P-\alpha_{10}}{\sqrt{\mu_{20}}}\right)^2+\left(\frac{Q-\alpha_{01}}{\sqrt{\mu_{02}}}\right)^2.$$

From the phase-space representative of this commutation relation the Poisson bracket

$$(A(p,q),\,\varrho(p,q))=0$$

is obtained. This equation has the solution

$$\varrho(p,q)=f(A(p,q))$$

and hence (15) is equivalent to the differential equation

$$f(A)+2\,\frac{df}{dA}=0$$

with the normalized solution

$$f(A)=2\,e^{-\frac{A}{2}}.$$

The distribution of minimum dispersion is thus given by

$$\varrho(p,q)=2\,e^{-\frac{1}{2}\left\{\left(\frac{p-\alpha_{10}}{\sqrt{\mu_{20}}}\right)^2+\left(\frac{q-\alpha_{01}}{\sqrt{\mu_{02}}}\right)^2\right\}}$$

with $\sqrt{\mu_{20}\,\mu_{02}}=\hbar/2$.

If $\varrho_1(p,q)$ and $\varrho_2(p,q)$ represent orthogonal states we have $(\varrho_1|\varrho_2)=0$ and if e.g. $\varrho_1(p,q)>0$ in every point, $\varrho_2(p,q)$ must certainly be negative somewhere in R_{2n}. This is the most remarkable difference between the quantum and the classical phase distribution. It is, however, not astonishing since the quantum distribution is not a probability distribution. But

$$\int \varrho(p,q)\,\frac{1}{h^n}\,dp=\langle q|\varrho|q\rangle\geq 0$$

$$\int \varrho(p,q)\,\frac{1}{h^n}\,dq=\langle p|\varrho|p\rangle\geq 0$$

are of course ordinary probability densities.

In complete analogy to Section 2 the equation of motion may be written as a differential equation for a unitary operator $\Lambda(t)$ belonging to the group $\mathbf{U}$

$$\frac{1}{i}\,\mathcal{H}[H]\,\Lambda(t)=\frac{d}{dt}\Lambda(t), \quad \Lambda(0)=1$$

where H is the Hamiltonian operator of the system. The time dependence may be attributed to the observables or to the states alternatively.

Eigenvalue equations in the state-vector space Hi may also be written as eigenvalue equations in $\mathcal{A}_2$. E.g. the energy eigenstates are determined from

$$\tfrac{1}{2}(H\varrho + \varrho H) = H'\varrho^1$$

with the subsidiary condition that ϱ shall be a projection operator. In $\mathcal{A}_1$ the same equation reads

$$\cos\left\{\frac{\hbar}{2}\sum_{\mu=1}^{n}\left(\frac{\partial}{\partial q'_\mu}\frac{\partial}{\partial p_\mu} - \frac{\partial}{\partial p'_\mu}\frac{\partial}{\partial q_\mu}\right)\right\} H(p', q')\,\varrho(p, q) = H'\varrho(p, q).$$

If $H(p, q)$ is a polynomial, the differential operator terminates and the quantum mechanical problem is equivalent to a differential equation in R_{2n}.

As an example we consider the Hamiltonian of the one-dimensional harmonic oscillator $H = (1/2\hbar\omega)(p^2 + \omega^2 q^2)$. Now H must commute with ϱ and

$$(p, q\,|\,\frac{1}{i\hbar}(H\varrho - \varrho H)) = (H(p, q), \varrho(p, q)) = 0.$$

It follows that $\varrho(p, q) = f(H(p, q))$ and the differential equation for $f(H)$ is

$$\left\{H - \tfrac{1}{4}\frac{d}{dH} - \tfrac{1}{4}H\frac{d^2}{dH^2}\right\} f(H) = H' f(H).$$

With the transformation $f(H) = e^{-2H}\psi(H)$ the equation reads

$$\left(H\frac{d}{dH} - \tfrac{1}{4}H\frac{d^2}{dH^2}\right)\psi(H) = (H' - \tfrac{1}{2})\,\psi(H).$$

The solution of this equation is $\psi(H) = L_{H'-1/2}(4H)$, where $L_n(x)$ are the Laguerre polynomials of zero order. Hence

$$\begin{aligned} f_{1/2}(H) &= 2\,e^{-2H} \\ f_{3/2}(H) &= 2(1 - 4H)\,e^{-2H} \text{ etc.} \\ &\ldots \end{aligned}$$

Obviously every distribution except for the ground-state is negative somewhere in R_{2n}. From the general properties of Laguerre polynomials follows the orthonormality of the different states

$$(\varrho_{H'}\,|\,\varrho_{H''}) = \delta(H', H'').$$

The ground state $\varrho_{1/2}(p, q) = 2\exp - ([p^2 + \omega^2 q^2]/\hbar\omega)$ is a normal distribution with

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[1] It is obvious that (HA) and $(HA + AH)$ are hermitean operations in $\mathcal{A}_2$ if H is a hermitean operator in Hi and A is an element of $\mathcal{A}_2$.

minimum dispersion since

$$\mu_{20}=\frac{\hbar\,\omega}{2},\quad \mu_{02}=\frac{\hbar}{2\,\omega}$$

and hence

$$\mu_{20}\,\mu_{02}=\left(\frac{\hbar}{2}\right)^2.$$

Mathematical statistics is built on the assumption of non-negative probability. It is obvious that the occurrence of negative "probabilities" is incompatible with the usual interpretation of probabilities as limits of frequency ratios. Nevertheless it would be of great interest to find out how far the general theorems of statistics (as e.g. the central limit theorem) are valid also for "negative probability distributions" subject to condition (14). It might be expected that generalized statistics of this kind could be useful for the exploitation of the ergodic theorems of classical mechanics in quantum mechanics.

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